

Abstract

Methods are disclosed for establishing a quantitative relationship between spectral properties of molecules and a biological, chemical, or physical endpoint of the molecules. Spectral data including data from nuclear magnetic resonance, mass spectrometric, infrared, and ultraviolet-visible techniques are used along with endpoint data to train a pattern-recognition program. The training yields a spectral data-activity relationship that may be used to predict the endpoint value of a molecule from its spectral data alone. Methods for rapidly screening isolated compounds or mixtures of compounds based upon their spectral data are included.